#### **CONCEPT: INTRO TO CRYSTAL FIELD THEORY**

- Transition metal coordination compounds form crystalline solids.
- Crystal field theory was developed to explain \_\_\_\_\_ and \_\_\_\_ properties of coordination compounds.
  - □ Focuses on the effects of ligands' electric field around the metal cation.



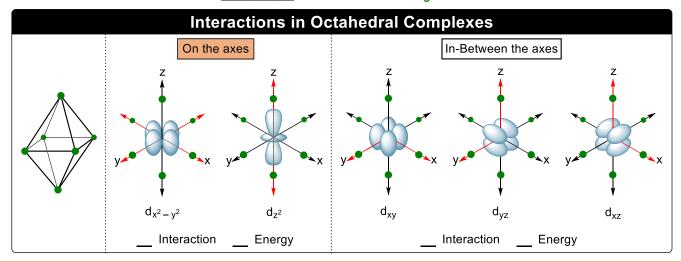
# **Ligand-Orbital Interactions**

- The interaction between the ligand and the metal cation is \_\_\_\_\_.
  - □ Increases the \_\_\_\_\_ of metal d orbitals: \_\_\_\_ interaction = \_\_\_\_ energy

Metal d orbitals ligand
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## **Interactions in Octahedral Complexes**

- The strength of ligand-orbital interaction depends on complex \_\_\_\_\_ and d orbital \_\_\_\_\_.
- Octahedral complexes: ligands are on the axes.
  - □ On the axes orbitals have the \_\_\_\_\_ interactions with the ligands.



**EXAMPLE**: Which set of d orbitals below will interact the most with the NH<sub>3</sub> ligands in [Fe(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>3</sub>?

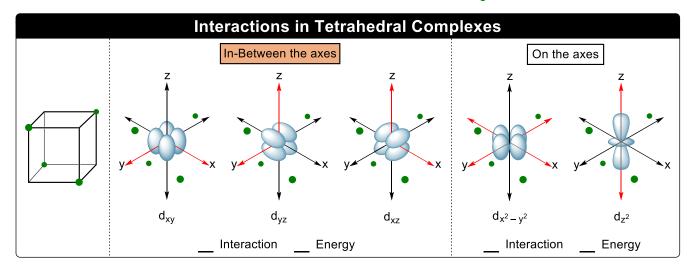
- $a)\;d_{xy},\,d_{yz},\,d_{xz}$
- b)  $d_{xy}$ ,  $d_{yz}$ ,  $d_x^2-y^2$
- c)  $d_{xz}$ ,  $d_{yz}$ ,  $d_z^2$
- d)  $d_{xy}$ ,  $d_x^2-y^2$ ,  $d_z^2$
- e)  $d_{x^{2}-v^{2}}$ ,  $d_{z^{2}}$

#### **CONCEPT: INTRO TO CRYSTAL FIELD THEORY**

## **Interactions in Tetrahedral Complexes**

• Tetrahedral complexes: ligands are aligned \_\_\_\_\_\_ the axes.

□ In-between the axes orbitals have the \_\_\_\_\_ interactions with the ligands.



**EXAMPLE**: Identify the d orbital(s) with the highest energy in the complex shown below?

a) d<sub>xy</sub>

b) d<sub>yz</sub>

c) d<sub>xz</sub>

d)  $d_z^2$ 

e)  $d_{x^{2}-v^{2}}$ 

f) both d and e g) a, b, and c

PRACTICE: For an octahedral complex, which set of d orbitals is expected to be at the lowest energy?

a) 
$$d_{xy}$$
,  $d_{yz}$ ,  $d_z^2$ 

b) 
$$d_{yz}$$
,  $d_{xz}$ ,  $d_z^2$ 

c) 
$$d_{xy}$$
,  $d_{yz}$ ,  $d_{xz}$ 

d) 
$$d_{xy}$$
,  $d_{yz}$ ,  $d_x^2-y^2$ 

e) 
$$d_{yz}$$
,  $d_x^2-y^2$ ,  $d_z^2$